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On the Structure of Self-Similar Detonation Waves in TNT Charges

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ABSTRACT

A phase plane method is proposed to model flow fields bounded by constant-velocity detonation waves propagating in TNT charges. Similarity transformations are used to formulate the problem in the phase plane of non-dimensional sound speed: Z versus non-dimensional velocity: F. The formulation results in two coupled ordinary differential equations that are solved simultaneously. The solution corresponds to an integral curve Z(F) in the phase plane, starting at the Chapman-Jouguet (CJ) point and terminating at singularity A—the sonic point within the wave. The system is closed by computing thermodynamic variables along the expansion isentrope passing through the CJ point—forming, in effect, the complete equation of state of the thermodynamic system. The CJ condition and isentropic states were computed by the thermodynamic code Cheetah. Solutions were developed for planar, cylindrical and spherical detonations. Species profiles were also computed; carbon graphite was found to be the predominant component (\sim 10 moles/kg). The similarity solution was used to initialize a 1D gas-dynamic simulation that predicted the initial expansion of the detonation products and the formation of a blast wave in air. Such simulations provide insight into the thermodynamic states and species that create the initial optical emissions from TNT fireballs.

Keywords: detonation waves in TNT, phase-plane method, similarity solution, CJ conditions, species

Nomenclature

Variables:
temperature: Tpressure: prelative energy: eabsolute energy: udensity: ρ sound speed: adetonation velocity: Wisentropic gamma: $\Gamma = (\partial \ln p / \partial \ln \rho)_s$ molar concentration of i^{th} species: C_i heat of detonation: ΔH_d radial velocity: \mathbf{u}_s

radial coordinate: rtime: tflow area: \mathcal{M} mass integral: \mathcal{M} energy integral: \mathcal{E} Non-dimensional variables: $\Theta = T / T_{CJ}$ $P = p / p_{CJ}$ $E = e / e_{CJ}$ $R = \rho / \rho_{CJ}$ $A = (a / a_{CJ})^2$

$$G = \Gamma / \Gamma_{CJ}$$

$$F = \mathbf{u}_r / xW_{CJ}$$

$$Z = a^2 / x^2W_{CJ}^2$$

$$U = \mathbf{u}_r / \mathbf{u}_{CJ} = xF / F_{CJ}$$

$$x = r / r_{CJ}$$

$$j = d \ln \mathcal{L} / d \ln r = 0, 1, 2$$

$$D = Z - (1 - F)^2$$

$$k_j = 4\pi, 2\pi \text{ and } 1 \text{ for } j = 2, 1, 0$$

$$h = \rho / \rho_0$$

$$g = p / \rho_0 W_{CJ}^2$$
subscripts:

Chapman-Jouguet state: CJ
constant energy and volume: UV
Reactants: R
Products: P
Standard Conditions (1 atm, 300 K): O

1. Introduction

Application of similarity methods to model explosions has a long and prestigious history. In 1941 Sir Geoffrey Taylor used a similarity variable to transform the partial differential equations of gas dynamics to the ordinary differential equations of blast wave theory [1], [2]. He used an equation of state for the TNT detonation products as developed by Jones and Miller [3]. He computed the pressure and velocity profiles behind the detonation front for planar and spherical waves [1], [2]; he showed for the first time, that in velocity was quiescent (zero) for the inner half of the detonation wave. He published additional studies of TNT detonations in the 1958 Princeton series on high-speed aerodynamics [2]. This similarity approach was formalized as the Phase Space Method by Academician Leonid Ivanovich Sedov in 1958 in his monograph Similarity and Dimensional Analysis in Mechanics [4]; he applied it to a wide variety of explosion and implosion problems. In 1960 Stanyukovich used similarity methods to model the escape detonation products into a vacuum [5]; the products were modeled by an isentropic power law ($\Gamma = 3$). G. I. Barenblatt has developed scaling methods [6] and extended the similarity method to the intermediate asymptotics regime [7]. A general description of the theory of detonation waves can be found in the treatise by Academician Yacob Borisovich Zel'dovich and Kompaneets [8]. A recent comprehensive review can be found in John Lee's book *The Detonation Phenomenon* [9].

Similarity methods enjoyed perhaps their greatest popularity in modeling explosions in gases—rather than solids¹. Oppenheim and coworkers used the Phase Space Method to derive all possible solutions bounded by a strong shock [10] or a strong detonation [11], detonations with variable energy at the front [12], pressure waves generated by steady flames [13] and blast waves in exponential atmospheres [14].

In this paper we develop a Phase Space Model for detonation waves in solids that accommodates a thermodynamically complete model of TNT detonation products based on the Cheetah thermodynamic code of Fried [15]. The thermodynamic properties of TNT are described in §2; the phase plane model is presented in §3; results are put forth in §4, including species profiles; this is followed by §5-Discussion and §6-Conclusions.

2. Thermodynamics of TNT detonations

The energetics of TNT detonation products are described by the locus of states in the Le Chatelier plane of specific internal energy: u versus temperature: T (see Fig. 1). The locus starts at the Chapman-Jouguet point: CJ and expands down the isentrope to 300 K; both the

¹ This is due to the fact gases can be accurately modeled as having a constant ratio of specific heats: γ , while detonation products from solid explosives require more complicated equations of state (e.g., JWL model) which have been outside the scope of the formulation of most similarity methods.

locus and the CJ condition itself were predicted by the Cheetah code.

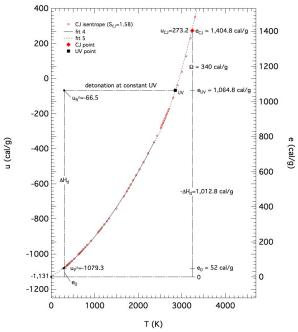


Figure 1. Le Chatelier diagram showing the expansion of TNT products from the CJ point to zero temperature. Note that the absolute and relative energy scales are related by $e = u+1,131 \, cal/g$. The solution also illustrates the energy jump condition across the detonation front: $e_{CJ} = e_0 + |\Delta H_d| + \Omega$; here $\Omega = W_{CJ}^2 / 2(\Gamma + 1)^2$ represents the kinetic-energy flux across the front.

The computed points (circles) are accurately fit with a piece-wise quadratic functions: $u_i(T) = a_i T^2 + b_i T + c_i$ as shown in Fig. 1. Fitting constants are listed in Table 1. In Fig. 1, the fundamental energy variable is u, which represents the absolute specific internal energy (that includes the heats of formation of the TNT molecules). On this scale, the Reactants and Products energies at 300 K are $u_R^0 = -66.5 \, cal/g$ and $u_P^0 = -1,079.3 \, cal/g$, respectively. Their difference represents the heat of detonation: $\Delta H_d = u_R^0 - u_P^0 = 1,012.8 \, cal/g$. This value is in

good agreement the heat of detonation of TNT: $1,093 \pm 1 \, cal/g \, cal/g \, (for \, \rho_0 = 1.533 \, g/cc)$ as measured by Ornellas in bomb calorimeter experiments [16]. On this scale, the value of energy at zero temperature is u(0) = -1.131 cal/g, indicating that the DP gases retain energy of $e_0 = 52 \, cal/g$ at room temperature. Figure 1 has an auxiliary energy scale: e that has the property that energy is zero at zero temperature. It is related to the absolute energy scale by: $e = u + 1{,}131$. Also shown in Fig. 1 is the detonation at constant energy and volume, denoted by point UV. On the e energy scale. the heat detonation of is: $\Delta H_d = e_{UV} - e_0 = 1,012.8 \, cal \, / \, g$. The enhancement from UV point to the CJ point is caused by the kinetic energy flux across the detonation front: $\Omega = W_{CJ}^2 / 2(\Gamma + 1)^2 = 340 \, cal / g$, where W_{CI} is the detonation wave velocity. One sees that the energy at the CJ point equals 273.2 cal/g and 1,404.8 cal/g on the absolute and the auxiliary energy scales, respectively. Thus, the energy characteristics of the TNT products gases are completely characterized by the Le Chatelier diagram of Fig. 1. Other thermodynamic variables were also

calculated along the CJ isentrope; they were non-dimensionalized by their values at the CJ point: Temperature: $\Theta = T / T_{CI}$; pressure: $E = e / e_{CI}$; $P = p / p_{CI}$; energy: density: $R = \rho / \rho_{CL}$; sound speed: $A = (a / a_{CL})^2$; and isentropic exponent: $G = \Gamma / \Gamma_{CI}$ (see Table 2 for the CJ values). Their inter-relationship is illustrated in Fig. 2 as a function of density ratio: R^2 along the CJ isentrope. We emphasize that this thermodynamic solution is general (e.g., devoid of any constant Γ assumptions, etc.). It is found by minimizing the Gibbs free

² The choice of R as the ordinate is appropriate because R will be shown to be one of the two dependent variables of the present phase plane model formulation, as shown in §3.

energy of the thermodynamic system for TNT. Thus by construction, it automatically satisfies the First Law of Thermodynamics along the CJ isentrope. Under such circumstances, use of the energy conservation law of gas dynamics becomes redundant (superfluous).

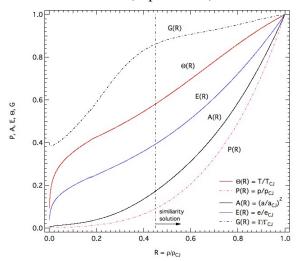


Figure 2. Non-dimensional relationship between thermodynamic variables along the CJ isentrope $(S_{CJ} = 1.58 \, cal \, / \, g - K)$ for TNT.

The corresponding species concentrations in the TNT detonation products are presented in Fig. 3 as a function of temperature. One can see that carbon graphite is the predominant component, followed by carbon monoxide and dioxide, diatomic nitrogen, water and methane. This solution: $C_i = f_i(T, S_{CJ})$, combined with the similarity solution, will be used to speciate the detonation wave.

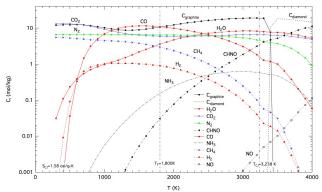


Figure 3. Species concentrations in the TNT detonation products along the CJ isentrope.

3. Phase Plane Model

We assume that the charge is initiated at r = t = 0, and consumed by a constant-velocity detonation, propagating at velocity W_{CJ} and satisfying the CJ jump conditions. The trajectory of the detonation front then obeys the linear relation:

$$r_{CI} = W_{CI} \cdot t_{CI} \tag{1}$$

Under such circumstances, time and space coordinates are related

$$dt = dr / W_{CI} \tag{2}$$

so one may define a similarity variable [10-11]:

$$x = r / r_{CI} \tag{3}$$

One may then transform the partial differential equations of gas dynamics into ordinary differential equations of blast wave theory that are a function of the similarity variable x [18]. It is useful to define the following phase plane variables:

$$F = \frac{u}{xW_{CI}} \qquad \& \qquad Z = \frac{a^2}{x^2W_{CI}^2} \tag{4}$$

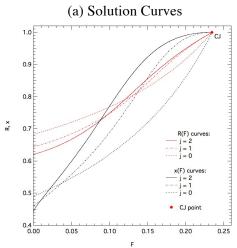
As shown in the Appendix, the governing equations may be arranged into two coupled ordinary differential equations (ODE's) for the dependent variables x and R as a function of the independent variable F:

$$\frac{d\ln x}{dF} = \frac{-1}{F} \frac{x^{-2}A(R) \cdot Z_{CJ} - (1 - F)^2}{(j + 1)x^{-2}A(R) \cdot Z_{CJ} - (1 - F)^2}$$
 (5)

$$\frac{d \ln R}{dF} = \frac{j(1-F)}{(j+1)x^{-2}A(R) \cdot Z_{CJ} - (1-F)^2}$$
 (6)

These are supplemented by the equation of state function: A(R) shown in Fig. 2. Here the

geometric index j equals 0, 1, or 2 for plane-, line- or point-symmetric flow, respectively. These equations are to be integrated from the CJ point in the phase plane: $\{F_{CJ} = 1/(\Gamma + 1); Z_{CJ} = [\Gamma/(\Gamma + 1)]^2\}$ where x = R = 1, to the singularity A located at $\{F = 0; Z = 1\}$. The solution curves x(F) and R(F) are presented in Fig. 4a for plane, line and point-symmetric flows; their corresponding curves are shown in the Z-F phase plane in Fig. 4b. The planar case represents a singular solution: $Z = (1 - F)^2$ lying along the D = 0; its solution can be found in [11].



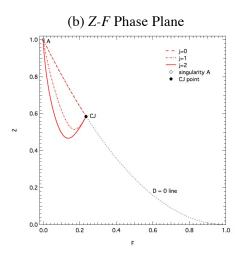


Figure 4. Similarity solutions for planar (j = 0), cylindrical (j = 1) and spherical (j = 2) Chapman-Jouguet detonation waves in TNT; (a) R-F and x-F plane, (b) Z-F plane.

4. Solution

One can invert the solution of (5) yielding F(x); combined with the solution of (6) one finds:

$$u/u_{CJ} = U(x) = x \cdot F(x)/F_{CJ} \tag{7}$$

$$\rho / \rho_{CJ} = R(F(x)) \tag{8}$$

So, the velocity and density profiles come directly from the solution curves x(F) and respectively. The thermodynamic R(F), profiles come from those solutions, as expressed through the equation of state relations $P = P(R), \Theta = \Theta(R), E = E(R), A = A(R), G = G(R)$ depicted in Fig. 2. The flow field profiles behind planar, cylindrical and spherical Chapman-Jouguet detonations propagating in charges are presented in Fig. 5. One can see that the velocity field goes to zero at $x \sim 0.5$ (the location of singularity A); inside that point, the flow is quiescent³ and the thermodynamic variables are constant. For spherical and cylindrical cases, the slope of the flow field profiles becomes infinite as one approaches the front. This is a consequence of the CJ boundary condition being located on the singular line $D = 0^4$. Also note that the isentropic index is not constant; it decreases to $G(x < 0.5) \sim 0.8$ behind the front.

Using the temperature field T(x) and the species functions $C_i(T)$, one can calculate the species fields $C_i(x)$; results are presented in Fig. 6 for the spherical case. The species concentrations change behind the front, in response to the temperature decay. Also notable is the electron concentration profile; this was computed from the carbon-graphite concentration and temperature Ershov [18].

³ As first predicted by G. I. Taylor in 1941 and 1950 [1].

⁴ Appendix, $d \ln F / d \ln x = -(jZ + D) / D \rightarrow \infty$ at D = 0

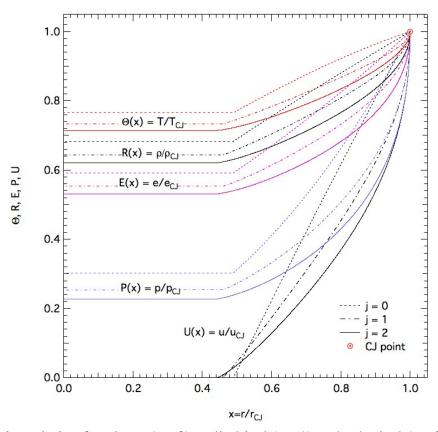


Figure 5. Similarity solution for planar (j = 0), cylindrical (j = 1) and spherical (j = 2) Chapman-Jouguet detonation waves in TNT.

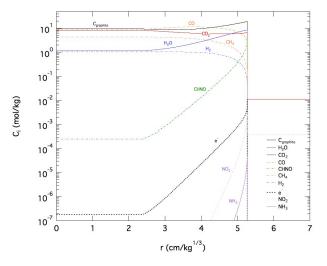


Figure 6. Species profiles in the TNT detonation products gases in a spherical CJ detonation.

5. Discussion

5.1 Mass and Energy Integrals

It is important to check that the solution (Fig. 5) actually conserves mass and energy. To that end we define the mass integral: \mathcal{U} and total energy integral: \mathcal{E} according to the following:

$$\mathcal{M}_{j} = k_{j} \int_{0}^{R_{c}} \rho_{j}(r) r^{2} dr \tag{9}$$

$$\mathcal{E}_{j} = k_{j} \int_{0}^{R_{c}} [e_{j}(r) + u_{r,j}^{2}(r)/2] \rho_{j}(r) r^{j} dr$$
 (10)

where R_c is the radius of charge, e is the relative energy and $k_j = 4\pi, 2\pi$ and 1 for j = 2, 1 and 0. The above integrals were computed with a

second-order quadrature method. Mesh refine studies indicated convergence when 10⁴ mesh points were used. Results for a 1-kg TNT charge $(R_c = 5.24556 \text{ cm}/\text{kg}^{1/3})$ are listed in Table 3. Mass errors ranged from -0.05% to +0.009%(-0.5 g to +0.06 g). Energy errors ranged from 0.14% to 0.18% (corresponding to 1.5 to 1.9 cal/g). We consider this to be adequate accuracy, considering that the solution functions must be represented on a finite grid, and the slopes of the profiles are infinite at the front. Also shown in Table 3 are peak values of e, Tand ρ (on the computational mesh) compared to the CJ state. It is this flow field that will be used to initialize a one-dimensional (1D) blast wave calculation in §5.3.

5.2 Constant-Gamma Solution

In contrast to the current work, previous studies assumed the gas to be a perfect with a constant ratio of specific heats: γ ; also, since the entropy varied in the blast wave, the isentropic assumption was not applicable, and the total energy conservation of gas dynamics was needed. Under these circumstances, the phase space method gave a single ordinary differential equation [19]

$$\frac{d\log Z}{d\log F} = \frac{2D + j(\gamma - 1)(1 - F)F}{jZ + D} \tag{11}$$

whose solution produced an integral curve in the Z-F phase plane. This was completed by:

$$\frac{d\log x}{d\log F} = \frac{-D}{jZ + D} \tag{12}$$

whose quadrature produced the auxiliary function x(F) [19]. These are supplemented by the definitions

$$u/u_{CJ} = x F/F_{CJ} \& T/T_{CJ} = x^2 Z/Z_{CJ}$$
 (13)

and the constant-gamma relations

$$\rho / \rho_{CJ} = (T / T_{CJ})^{1/(\gamma - 1)} \& p / p_{CJ} = (\rho / \rho_{CJ})^{\gamma}$$
 (14)

Equations (11)-(12) were integrated from the CJ point to singularity A for $\gamma = \Gamma_{CJ} = 3.2586$ and j = 2. The resulting solution profiles are presented in Fig. 7 and compared to the variable Γ solution of the previous section (Fig. 5). The two solutions are similar but different; all profiles for the constant Γ case lie above the variable Γ profiles; this results in irreducible errors in the global mass and energy integrals. Table 3 indicates a mass error of +1.1% and energy error of +1.9% for the constant- Γ solution.

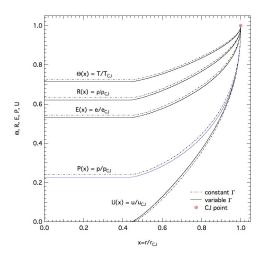


Figure 7. Comparison of the Γ =3.2586 solution versus the CJ-isentrope solution (S = 1.58 cal/g-K) for the spherical case (j = 2). The constant- Γ model introduces a +1.1 % error in mass: \mathcal{M}_2 and a +1.9% error in total energy: \mathcal{E}_2 .

5.3 Species profiles in TNT blast wave in air

The variable- Γ similarity solution for a spherical CJ detonation wave in TNT was used to initialize a 1D gas dynamic code simulation. The species waveforms in the TNT detonation products gases at t = 0 and 2.5 μ s are presented in Fig. 8. There we see the preponderance of

carbon graphite (9.9 moles), CO_2 (8.9 moles) and CO (7.5 moles) over CH_4 (4.5 moles) H_2 (1 mole) and H_2O (1 mole) at the early stages of expansion of the detonation products gases at $t = 2.5 \, \mu s$.

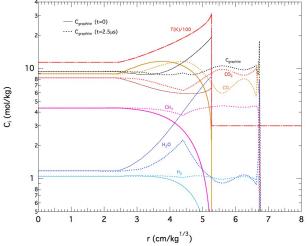


Figure 8. Species waveforms in the TNT detonation products gases at t = 0 and 2.5 μs in a spherical CJ detonation wave.

8. Conclusions

A phase plane model is proposed to describe flow fields bounded by CJ detonation waves in spherical, cylindrical and planar symmetries. The model is based on two coupled ODE's for $d \ln x / dF$ and $d \ln R / dF$. The system is closed by thermodynamic relations: P(R), $\Theta(R)$, E(R), A(R), G(R) and $C_i(T)$ corresponding to the equilibrium solution along the CJ isentrope for the considered thermodynamic system. In effect, they enforce energy conservation along the isentrope—thereby eliminating the need to employ the energy conservation equation of gas dynamics for this particular problem. The solution of the ODE's prescribes the functions x(F) and R(F), which then specify the velocity U(x) and density R(x) profiles behind the front. Used in conjunction with the thermodynamic relations, they also prescribe the thermodynamic P(x), $\Theta(x)$, E(x), A(x) and $C_i(x)$ profiles: behind the front. The predicted solution conserves global mass (within 0.05%) and global energy (within 0.2%) on the computational grid employed for the integrals (10^4 cells).

The present formulation reveals (brings to the surface) the central role played by the internal energy locus: u(T) in the Le Chatelier plane (Fig. 1). Not only does it uniquely relate internal energy and temperature, it completely specifies the caloric relations of the system. And the CJ point itself possesses almost magical properties: (i) not only does it specify the jump conditions across the detonation front, (ii) it controls the mass and energy conservation behind the front, and (iii) it is itself a singularity of the ODE system—causing the slope of the flow field profiles to become infinite at the front.

Such simulations provide unique insight into the thermodynamic states and species that create optical emissions from TNT fireballs. This approach should be used to study the structure and emission properties of detonation waves in other HE charges.

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Appendix:

Derivation of the Phase Plane Equations

From our previous paper on the systematic exposition of the conservation equations of blast waves [14], one finds

$$-D\frac{d\ln F}{d\ln x} = D + jZ = (j+1)Z - (1-F)^2$$
 (A1)

$$-D\frac{d\ln h}{d\ln x} = \frac{F}{1-F}[D+jZ-(j+1)D] = jF(1-F)$$
(A2)

where $Z = x^{-2}\Gamma g/h$ with $g = p/\rho_0 W_{CJ}^2$ and $h = \rho/\rho_0$, and where $D = Z - (1-F)^2$. Re-write in terms of F as the independent variable, and changing from h to $R = \rho/\rho_{CJ}$ on finds:

$$\frac{d\ln x}{dF} = \frac{-1}{F} \frac{Z - (1 - F)^2}{(j + 1)Z - (1 - F)^2}$$
 (A3)

$$\frac{d\ln R}{dF} = \frac{j(1-F)}{(j+1)Z - (1-F)^2}$$
 (A4)

Now express Z by $Z = x^{-2}A \cdot Z_{CJ}$ where $A = (a/a_{CJ})^2$ denotes the non-dimensional sound-speed squared and is a function of R from the thermodynamic solution along the CJ insentrope (i.e., A = A(R) as shown in Fig. 2). Then the above become two coupled ordinary differential equations:

$$\frac{d\ln x}{dF} = \frac{-1}{F} \frac{x^{-2} A(R) \cdot Z_{CJ} - (1 - F)^2}{(j + 1)x^{-2} A(R) \cdot Z_{CJ} - (1 - F)^2}$$
(A5)

$$\frac{d \ln R}{dF} = \frac{j(1-F)}{(j+1)x^{-2}A(R) \cdot Z_{CI} - (1-F)^2}$$
 (A6)

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These are to be integrated over the domain $0 < F \le F_{CJ}$.

The planar case (j = 0) is singular; the integral curve is the D = 0 line, thereby specifying a closed form solution [11]:

$$Z = (1 - F)^{2} & x = \frac{1 - (\Gamma + 1)F_{CJ}/2}{1 - (\Gamma + 1)F/2}$$
 (A7)

Tables

Table 1 Quadratic fits to the TNT locus: $u_i(T) = a_i T^2 + b_i T + c_i$

	Region i	a_i	b_{i}	C_{i}
Fi	300 < T < 2357	6.9982×10 ⁻³	0.16051	-1,131
t				
4				
Fi	2118 < T < 3700	35.227×10 ⁻⁵	-1.2316	579
t				
5				

Table 2 CJ and UV states for TNT ($\rho_0 = 1.654 \ g/cc$)

Variable	CJ State	UV State
p(kbar)	197.59759	90.13
$\rho(g/cm^3)$	2.1616	1.654
e(cal/g)*	1,352.46	1,064.8
u(cal/g)	273.16	-66.5
T(K)	3,237.875	2,866.9
s(cal/g-K)	1.58447	1.623
$\mathbf{u}_r(km/s)$	1.68595	0
W(km/s)	7.18	0
a(km/s)	5.4939	4.0593
$\Gamma = W_{CJ} / \mathbf{u}_{r,CJ} - 1$	3.2586	_

^{*} e = u + 1,131

Table 3
Solution Accuracy versus Theory for TNT
Detonation Waves

Varia	Thee	Similarity Solution			Γ=3.2
	Theo ry				5
ble		j = 0	j = 1	j = 2	j = 2
\mathcal{M}_0	1.000	1.000	0.999	1.000	1.011
(kg)	0	06	47	09	65
\mathcal{E}_0	1,064	1,063.	1,062.	1,062.	1,085.
(cal/g)	.8	3	3	9	5
peak e	1,404	1,402.	1,391.	1,386.	1,387.
(cal/g)	.8	5	3	9	6
peak	3,237	3,227.	3,216.	3,212.	3,213.
T(K)	.9	4	5	3	0
peak	2.161	2.161	2.148	2.140	2.141
ρ	6	2	5	5	5
(g/cc)					